

Claims

- [c1] A method for chemical compound development project management comprising:
 - providing a molecule database wherein records of the molecule database include molecular information regarding reactants and products of the synthesis steps required to produce an identified target molecule;
 - providing a synthesis database wherein records of the synthesis database include activity information regarding activities to transition between the synthesis steps of the target molecule synthesis; and
 - deriving information regarding a chemical compound development project from the molecule database and from the synthesis database.
- [c2] The method of claim 1 wherein the step of deriving includes:
 - identifying, from the molecule database, materials required in production of the target molecule.
- [c3] The method of claim 2 wherein the step of deriving further includes:
 - generating a bill of materials identifying quantities of all materials required in production of the target molecule.

- [c4] The method of claim 1 wherein the step of deriving includes:
identifying, from the synthesis database, resources required in production of the target molecule.
- [c5] The method of claim 4 wherein the step of deriving further includes:
identifying, from the synthesis database, activities associated with the identified resources.
- [c6] The method of claim 5 wherein the step of deriving further includes:
generating a GANTT chart scheduling the identified resources and the identified activities in production of the target molecule.
- [c7] The method of claim 1 wherein the step of deriving includes:
identifying, from the molecule database, materials required in production of the target molecule;
identifying, from the synthesis database, resources required in production of 5 the target molecule;
identifying, from the synthesis database, costs associated with the identified materials and associated with the identified resources; and
generating an estimated project cost from the identified

costs.

- [c8] The method of claim 1 wherein the step of deriving includes:
searching the molecule database or the synthesis database using chemical indicia to retrieve information regarding a chemical compound development project.
- [c9] A method for chemical compound development project management comprising:
providing a molecule database wherein records of the molecule database include molecular information regarding reactants and products of the synthesis steps required to produce an identified target molecule; and providing a synthesis database wherein records of the synthesis database include activity information regarding activities to transition between the synthesis steps of the target molecule synthesis; and generating a synthesis plan for a target molecule using molecular information from the molecule database and using activity information from the synthesis database.
- [c10] The method of claim 9 wherein the step of generating includes:
identifying, from the molecule database, all intermediate molecules required in production of the target molecule.

- [c11] The method of claim 10 wherein the step of identifying all intermediate molecules includes:
identifying materials required for production of all intermediate molecules and production of the target molecule.
- [c12] The method of claim 11 wherein the step of generating further includes:
identifying, from the synthesis database, activities required for production of all intermediate molecules and for production of the target molecule.
- [c13] The method of claim 12 wherein the step of generating further includes:
identifying, from the synthesis database, resources required for production of all intermediate molecules and for production of the target molecule.
- [c14] The method of claim 13 wherein the step of generating further includes:
identifying, from the molecule database and from the synthesis database, costs associated with the identified materials and with the identified resource and with the identified activities required for production of all intermediate molecules and for production of the target molecule.

- [c15] The method of claim 9 further comprising:
 - estimating total costs to develop the target molecules;
 - and
 - generating an offer to develop the target molecule for a customer wherein the offer includes a price derived from the estimated total cost.
- [c16] The method of claim 15 further comprising:
 - receiving acceptance from the customer to develop the target molecule in accord with the offer; and
 - adding experiments to the synthesis plans to schedule resources required to develop the target molecule.
- [c17] The method of claim 16 further comprising:
 - tracking progress of the development of the target molecule based on progress of the experiments.
- [c18] A system for target chemical compound development comprising:
 - a molecule database including information regarding intermediate chemical compounds required to produce the target chemical compound;
 - a synthesis database including information regarding steps required to transition between the synthesis steps of the target molecule synthesis; and
 - a chemical compound development management system for generating project synthesis plans integrating infor-

mation from both the molecule database and the synthesis database.

- [c19] A system for chemical compound development project management comprising:
 - means for providing a molecule database wherein records of the molecule 10 database include molecular information regarding reactants and products of the synthesis steps required to produce an identified target molecule;
 - means for providing a synthesis database wherein records of the synthesis database include activity information regarding activities to transition between the synthesis steps of the target molecule synthesis; and
 - means for deriving information regarding a chemical compound development project from the molecule database and from the synthesis database.
- [c20] The system of claim 19 wherein the means for deriving includes:
 - means for identifying, from the molecule database, materials required in production of the target molecule.
- [c21] The system of claim 20 wherein the means for deriving further includes:
 - means for generating a bill of materials identifying quantities of all materials required in production of the

target molecule.

- [c22] The system of claim 19 wherein the means for deriving includes:
means for identifying, from the synthesis database, resources required in production of the target molecule.
- [c23] The system of claim 22 wherein the means for deriving further includes:
means for identifying, from the synthesis database, activities associated with the identified resources.
- [c24] The system of claim 23 wherein the means for deriving further includes:
means for generating a GANTT chart scheduling the identified resources and the identified activities in production of the target molecule.
- [c25] The system of claim 19 wherein the means for deriving includes:
identifying, from the molecule database, materials required in production of the target molecule;
identifying, from the synthesis database, resources required in production of the target molecule;
identifying, from the synthesis database, costs associated with the identified materials and associated with the identified resources; and

generating an estimated project cost from the identified costs.

- [c26] The system of claim 19 wherein the means for deriving includes:
means for searching the molecule database or the synthesis database using chemical indicia to retrieve information regarding a chemical compound development project.
- [c27] A computer readable storage medium tangibly embodying program instructions implementing a method for chemical compound development project management, the method comprising:
providing a molecule database wherein records of the molecule database include molecular information regarding reactants and products of the synthesis steps required to produce an identified target molecule;
providing a synthesis database wherein records of the synthesis database include activity information regarding activities to transition between the synthesis steps of the target molecule synthesis; and
deriving information regarding a chemical compound development project from the molecule database and from the synthesis database.
- [c28] The medium of claim 27 wherein the method step of de-

riving includes:
identifying, from the molecule database, materials required in production of the target molecule.

- [c29] The medium of claim 28 wherein the method step of deriving further includes:
generating a bill of materials identifying quantities of all materials required in production of the target molecule.
- [c30] The medium of claim 27 wherein the method step of deriving includes:
identifying, from the synthesis database, resources required in production of the target molecule.
- [c31] The medium of claim 30 wherein the method step of deriving further includes:
identifying, from the synthesis database, activities associated with the identified resources.
- [c32] The medium of claim 31 wherein the method step of deriving further includes:
generating a GANTT chart scheduling the identified resources and the identified activities in production of the target molecule.
- [c33] The medium of claim 27 wherein the method step of deriving includes:
identifying, from the molecule database, materials re-

quired in production of the target molecule; identifying, from the synthesis database, resources required in production of the target molecule; identifying, from the synthesis database, costs associated with the identified 25 materials and associated with the identified resources; and generating an estimated project cost from the identified costs.

- [c34] The medium of claim 27 wherein the method step of deriving includes:
searching the molecule database or the synthesis database using chemical indicia to retrieve information regarding a chemical compound development project.
- [c35] An interface for integrating various information management functions, the interface comprising computer readable program code devices for:
receiving a request to develop materials and procedures for a synthesis plan appropriate for manufacturing a particular desired chemical compound;
creating a new project synthesis plan entry in the project synthesis plan database correlating to the desired chemical compound;
accessing a molecule database to retrieve molecular information regarding reactants and products of synthesis steps required to produce the desired chemical com-

pound; accessing a synthesis database to retrieve activity information regarding activities to transition between the synthesis steps of the desired chemical compound synthesis; and deriving information regarding the chemical compound project synthesis plan from information retrieved from the molecule database and the synthesis database and adding steps and activities to the project synthesis plan.

- [c36] The interface as recited in claim 35 where the readable program code devices for deriving information includes identifying from the molecule database, material required in production of the desired chemical compound.
- [c37] The interface as recited in claim 36 where the readable program code devices for deriving information includes generating a bill of materials identifying quantities of all materials required in production of the desired chemical compound.
- [c38] The interface as recited in claim 35 where the readable program code devices for deriving information includes identifying from the synthesis database, resources required in production of the desired chemical compound.
- [c39] The interface as recited in claim 38 where the readable

program code devices for deriving information includes identifying from the synthesis database activities associated with identified resources.

- [c40] The interface as recited in claim 39 where the readable program code devices for deriving information includes generating a GANTT chart scheduling the identified resources and the identified activities in production of the desired molecule.
- [c41] A computer readable medium containing a data structure for storing data relevant to the management of chemical compound development and for integrating and sharing data to derive a project synthesis plan, the data structure comprising:
 - a project header data structure containing basic project information including a project identifier and a desired chemical compound; and
 - a synthesis plan data structure containing synthesis plans that can be correlated by the project identifier to the project header data structure and correlated by molecule identifiers and structures that reference to molecule data structures.
- [c42] The computer readable medium containing a data structure as recited in claim 41 where the synthesis plan data structure contains a project plan reference for referenc-

ing a project plan data structure containing specific steps and activities for developing the desired chemical compound.

- [c43] The computer readable medium containing a data structure as recited in claim 42 where the synthesis plan data structure contains a project estimate reference for referencing a project estimate data structure containing resource needs for each step and activity and material needs.